Numerical issues of the CFD-MC tokamak edge modelling

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Numerical simulations of the tokamak edge plasmas are crucial to analyze the loads on the Plasma Facing Components and impurity transport in present experiments as well as in the future tokamak fusion reactors. An approach which is often used for those simulations is a 2D fluid (CFD - Computational Fluid Dynamic) model for plasma (ions and electrons), coupled self-consistently with kinetic Monte-Carlo (MC) model for neutral particles. B2-EIRENE [1] is an example of the code package based of this approach. In very general terms, the problem solved by such code can be described as a set of algebraic equations:

$$\mathrm{F}(\phi) = S(\phi)$$

Where $\phi = \{n, u, T_e, T_i\}$ is the solution: density of ions and their average parallel velocity, electron and ion temperature; $\mathrm{F}(\phi)$ are the discretized equations for the parallel momentum, continuity (pressure correction), electron and ion energy balance; $S(\phi)$ are the particle, parallel momentum and energy sources due to interaction of charged and neutral particles - they are calculated by MC.

In practical calculations the time-marching relaxation scheme is typically used with MC model called on each time-iteration. That is, on each time-iteration k the following set of equations with respect to ϕ_k is solved:

$$\mathrm{F}(\phi_k) = \tilde{S}\left(\phi^m_{k-1}|\phi_k\right) + D\left(\phi_k, \phi^m_{k-1}\right) \tag{1}$$

Here ϕ^m_k is the approximate solution which comes out of the solver, $\tilde{S}\left(\phi^m_{k-1}|\phi^m_k\right)$ is the MC estimate of the source terms and $D\left(\phi_k, \phi^m_{k-1}\right)$ is the discrete time-derivative added to the equations. Notation $\left(\phi^m_{k-1}|\phi^m_k\right)$ means that the source is calculated for the "old" plasma ϕ^m_{k-1} but the modification of plasma parameters is partly taken into account.

Inserting the approximate solution ϕ^m_k back into Equation (1) yields common CFD residual:

$$R^m_k = \mathrm{F}(\phi^m_k) - \tilde{S}\left(\phi^m_{k-1}|\phi^m_k\right) - D\left(\phi^m_k, \phi^m_{k-1}\right)$$

This residual can be generalized for the CFD-MC combination:

$$\mathrm{F}(\phi^m_k) = S(\phi^m_k) + \tilde{R}, \quad \tilde{R} = R^m_k + \tilde{S}\left(\phi^m_{k-1}|\phi^m_k\right) - S(\phi^m_k) + D\left(\phi^m_k, \phi^m_{k-1}\right)$$

$$\left\|\tilde{R}\right\| \leq R+\Delta S \leq G = R+\Delta\tilde{S}+E\left(\Delta\tilde{S}\right), \quad R = \|R_k^m\|, \quad \Delta\tilde{S} = \left\|\tilde{S}\left(\phi_{k-1}^m|\phi_k^m\right) - \tilde{S}\left(\phi_k^m\right) + D\left(\phi_k^m, \phi_{k-1}^m\right)\right\| \tag{2}$$

Here $S\left(\phi_k^m\right)$ is the "exact" value of the source as it would be calculated with infinite number of MC particles. Since this exact value is not known in practice, only an estimated value of $\Delta\tilde{S}$ can be given, and $E\left(\Delta\tilde{S}\right)$ is the estimate of the statistical error of $\Delta\tilde{S}$. With l_1 norm the generalized residual G can be split into partial residuals for individual equations.

In ITER simulations performed with B2-EIRENE (SOLPS4.3) code [2] internal iterations are used to solve Equation (1). That is, discrete analog of each equation is written in the form of linear equations with coefficients dependent of ϕ. On each internal iteration j the sets of linear equations are solved with respect to ϕ (ϕ_k^j). Decision to accept or reject the final solution is based on empiric convergence criteria: steady state have to be reached, global particle and energy balances have to be fulfilled. Experience shows that m=15..20 internal iterations are required to get solutions converged in terms of those criteria.

Main drawback of internal iterations is that they restrict the type-step Δt - large values of Δt lead to numerical instability. Typical value for ITER simulations is $\Delta t \approx$1e-6 sec which translates into $\sim$1e5...1e6 time-iterations required for convergence meaning up to several months of wall-clock time for one model run.

Extensive studies has been initiated by EFDA in 2013 in order to reduce turn-around time of B2-EIRENE calculations for large machines (project WP13-SOL continued by EUROfusion WPDC-SOLPS-OPT). The run-time problem of a code like B2-EIRENE can not be considered separately from the numerical accuracy. Therefore, in frame of this project the iterative procedures of B2-EIRENE with different run-time have been compared for the reference ITER simulations in terms of accuracy of final solutions. The results are presented in the report [3]. A short summary of this study is presented below.

Apparently, the time-step can be increased up to $\Delta t \approx$1e-4 sec if no internal iterations: $m = 1$, are applied. However, in this case the steady-state solution obtained at the end may have very large error in the global particle balance, thus, it is not converged at all. Particle balance is very important because in the steady-state reactor discharges flux to the pump has to be equal to the sum of the gas puffing and core fueling rate - particle throughput. The upstream plasma pressure in the model (hence, density) is self-adjusted to ensure the required pumping rate by increasing/decreasing the divertor gas pressure. Therefore, error in the particle balance of the order of throughput can drive the solution into completely wrong direction.

The reason of wrong particle balance without internal iterations is found to be too large CFD residual R. Its reduction to acceptable level with m =1 may require massive - by a factor of 40 -

increase of the number of MC test particles. In order to solve the issue an intermediate type of internal iterations has been implemented: with one full internal iteration followed by iterating the continuity equations only - "continuity iterations". Continuity iterations, indeed, converge even with Δt=1e-4 sec, while bringing the error in the particle balance down to acceptable level.

Different iteration schemes can be compared in terms of generalized residual, Equation (2). Internal iterations are very efficient in reducing residual R making it negligible: $R << \Delta\tilde{S}$. With $m = 1$ the CFD residual is comparable to the second term: $R \sim \Delta\tilde{S}$. Both terms are reduced with increased number of MC particles. Continuity iterations, while making R for the particle balance equation very small, may lead to degradation of accuracy of other equations - especially of those for the parallel momentum balance, for which R becomes the dominant term: $R > \Delta\tilde{S}$.

Continuity iterations are found to be absolutely necessary at low particle throughput. In this cases the divertor plasma is nearly attached to divertor targets - parallel momentum losses due to ion-neutral friction are small. Degradation of accuracy of the momentum balance due to continuity iterations is moderate. The situation is different at high throughput, when divertor plasma is detached and momentum losses start to play very important role. Application of continuity iterations to this scenario leads to stronger increase of R (thus G) for momentum balance. Normalized G: divided by the norm of corresponding source term, can even get larger than 1. That is, roughly speaking, the error becomes larger than the physical source itself. Fortunately, at high throughput relative error in the global particle balance is found to be small enough even without extra correction. Therefore, continuity iterations may be omitted in the high throughput cases or applied only for selected species (e.g. He).

The effect which normalized $G \gtrsim 1$ can have on the final solution can only be estimated empirically by comparing runs made with different number of test particles, with $m = 1$ and $m > 1$. Tests have shown that even in high throughput case the solutions obtained with continuity iterations are always close to those calculated with full internal iterations and increased number of particles. Thus, a two-phase approach can be suggested for practical calculations. First phase is a fast run with large $\Delta t \approx$1e-4 sec, $m = 1$ and continuity iterations. Second phase is slow "refinement" performed with $m > 1$ and decreased $\Delta t \approx$1e-6 sec, or without continuity iterations but with (massively) increased number of test particles.

The next logical strep to resolve the both particle and momentum balance issues would be to extend continuity iterations and to iterate the coupled continuity and momentum balance equations after one full internal iteration. This algorithm - called "incomplete iterations" - has been tried as well and have not brought positive results so far. Incomplete iterations are found not to converge with large Δt, similar to the full internal iterations. One possible reason for this

might be rather primitive algorithm for pressure correction applied in the B2 code: compressible version of Patankar's SIMPLE, see [4], Chapter 6.7 and [5], Chapter 3. More advanced methods, such as Uzawa algorithm, should be tested in the future.

Estimating the efficiency of He pumping is one of the goals of the edge modelling for ITER, therefore, He ions are present as fluids in the model. While He is a trace-impurity which does not have big impact on the overall solution, its inclusion into the model poses extra numerical difficulties. Convergence of the He particle balance is slow and may even determine the total amount of time-iterations required to reach the steady-state solution. At the same time, wrong particle balance for He may lead to unphysically strong He radiation in front of divertor targets which significantly perturbs the solution. Introducing a separate model for the He transport applied on the post-processing stage can be suggested to ease the converges without compromising too much the physics accuracy of the model.

Fundamental problem of the CFD models with source terms calculated by Monte-Carlo is the absence of the solid estimate of the error in the solution itself. One would generally agree that generalized residuals G have to be made as small as possible, and the situation when for some equation normalized $G \sim 1$ can not be considered as satisfactory. Tests have shown that for ITER simulations an increase of the MC accuracy equivalent to approximately 100 fold increase of the number of MC test particles is required to obtain $G \lesssim 0.1$ for all equations. With such high accuracy it would be possible to make runs with $m = 1$ and $\Delta t \approx$1e-4 sec without special concern about the particle balance. The MC particle sampling can be easily parallelized and in B2-EIRENE simulations of ITER typically 32-64 CPUs are used for this part which makes the MC run-time comparable to that of the serial plasma fluid solver. Brute-force increase of the number of MC particles is, therefore, always possible technically but would require massive increase of computing power of a homogenous system. Alternatively, one could think of executing the runs on a heterogeneous system with MC running on GPU or ARM architecture.

References

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